

Association of heteronuclear molecules in a harmonic oscillator well

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(Dated: February 1, 2008)

We describe the collisional interaction between two different atoms that are trapped in a harmonic potential. The atoms are exposed to a magnetic field, which is modulated in the vicinity of an s-wave Feshbach resonance, and we study the formation of molecular bound states and excited states of the trapped system with non-trivial angular correlations.

PACS numbers: 03.75.Nt, 36.90.+f, 05.30.Jp, 05.30.Fk

I. INTRODUCTION

Among the variety of processes and phenomena that have been studied with degenerate quantum gasses, the conversion of an atomic Bose [1, 2, 3, 4] or Fermi-gas [4, 5, 6] of atoms into a gas consisting of diatomic molecules is one of the most fascinating, because the entire system undergoes a dramatic change of state and because it provides a practical way to produce a quantum degenerate state of a molecular species, which may not be reached easily in any other way. This process, which can be driven both by photo-association, by sweeping a B-field across a Feshbach collisional resonance in the system and by RF association from another hyperfine state, has been studied both in larger trapped samples where the collective many-body state changes character, and in the Mott insulating phase in optical lattices [7, 8, 9, 10, 11], where the process involves only two particles and can be understood microscopically.

With the association of different atomic species one has the possibility to form polar molecules, which offer interesting interaction dynamics both in large condensates [12, 13, 14, 15], and in Mott insulators, where the long range dipole-dipole interaction between molecules, e.g., makes them an interesting candidate for quantum simulators and quantum computers [16, 17]. In the present theoretical paper we study the dynamics of a pair of different atoms in the vicinity of an s-wave collisional resonance. We treat the case of atomic systems prepared in an optical lattice potential with precisely one atom pair per site, and we treat the case of a deep lattice well approximated by a harmonic potential. This system has recently been implemented and studied [7], and the production of molecules by RF association from another hyperfine state was demonstrated. We shall identify the eigenstates of the problem for different values of the B-field and solve the dynamical equations when the field is modulated. In particular we will show that oscillations of the field with a frequency which is resonant with the Bohr frequency between discrete atomic-like and molecular-like levels in the trapping potential offers unique opportunities for controllable transfer of the atoms to specific excited and molecular bound states in the trap.

In Sec II, we outline the basic theory, which is complicated here by the fact that the problem with different atoms does not separate in center-of-mass and relative coordinates. In Sec. III, we treat the atomic interaction by the conventional pseudo-potential, and we show that all necessary matrix elements of the Hamiltonian can be determined analytically, and the eigenstates and energies can be found by diagonalization of not too large matrices. The eigenstates have definite total angular momentum, but the non-separability implies that the states are not eigenstates of the separate center-of-mass and relative angular momentum. In Sec. IV we generalize our earlier dynamical calculations [18] to the heteronuclear case. Using a harmonic oscillation of the magnetic field we demonstrate association of heteronuclear molecules with 100 % efficiency and show that even though we start from spherically symmetric states and have only s-wave interaction and symmetric external potentials, it is possible to drive the system into states with non-zero relative angular momentum. Sec. V concludes the paper.

II. NON-SEPARABLE MOTION OF DIFFERENT ATOMS IN A HARMONIC POTENTIAL

If the potential depth in an isotropic 3-dimensional optical lattice, $V(\mathbf{r}) = V_0 \sum_{i=x,y,z} \sin^2(kx_i)$, is significantly larger than the tunnelling energy between lattice sites, atoms placed in the lattice may be prepared in a Mott-insulating state with a well defined number of atoms in each well. Provided that the lattice is also deeper than the recoil energy $\hbar^2 k^2 / 2m$, the atoms experience around each potential minimum a harmonic oscillator potential

$$V(\mathbf{r}) \simeq V_0 k^2 \sum_{i=x,y,z} x_i^2 = V_0 k^2 r^2 = \frac{1}{2} m \omega^2 r^2, \quad (1)$$

where $\omega = \sqrt{2V_0 k^2 / m}$, k is the optical wave number and m is the mass of each atom.

We shall treat the dynamics of two atoms, with masses m_1 and m_2 and position coordinates \mathbf{r}_1 and \mathbf{r}_2 , from

which we form the center-of-mass (CM) and relative coordinates

$$\mathbf{R} = \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2} \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2. \quad (2)$$

The Hamiltonian with an atomic interaction potential $V_{\text{int}}(\mathbf{r})$ reads

$$H = -\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + \frac{1}{2} m \omega_1^2 r_1^2 + \frac{1}{2} m \omega_2^2 r_2^2 + V_{\text{int}}(\mathbf{r}), \quad (3)$$

and it does not separate in center-of-mass and relative coordinates, but it can be rewritten

$$H = H_{\text{cm}}(\mathbf{R}) + H_{\text{rel}}(\mathbf{r}) + C \mathbf{R} \cdot \mathbf{r}, \quad (4)$$

with

$$H_{\text{cm}} = \frac{-\hbar^2}{2M} \nabla_{\mathbf{R}}^2 + \frac{1}{2} M \Omega^2 R^2 \quad (5)$$

$$H_{\text{rel}} = \frac{-\hbar^2}{2\mu} \nabla_{\mathbf{r}}^2 + \frac{1}{2} \mu \omega^2 r^2 + V_{\text{int}}(\mathbf{r}). \quad (6)$$

In (5), we have introduced the total and reduced masses $M = m_1 + m_2$, $\mu = m_1 m_2 / M$.

The frequencies Ω and ω and the coupling coefficient C have non-trivial values determined by equating the potential terms in (3) and (4),

$$\frac{\Omega}{\omega_1} = \sqrt{\frac{1+\beta}{1+\alpha}}, \quad \frac{\omega}{\omega_1} = \sqrt{\frac{\alpha+\beta/\alpha}{1+\alpha}}, \quad \frac{C}{m_1 \omega_1^2} = \frac{\alpha-\beta}{1+\alpha} \quad (7)$$

where we define the mass ratio $\alpha = m_2/m_1$ and the ratio of the harmonic oscillator depths $\beta = (m_2 \omega_2^2)/(m_1 \omega_1^2)$.

Note that in the case $\omega_2 = \omega_1$ (that is, $\alpha = \beta$) we have $\Omega = \omega = \omega_1 = \omega_2$ and $C = 0$ so the center-of-mass and relative motion separate exactly, independently of the masses. In the general case we obtain a simple $C \mathbf{R} \cdot \mathbf{r}$ coupling of the two degrees of freedom, which suggests to diagonalize this coupling in the factored basis of eigenstates of the separate problems.

Let us take ^{87}Rb and ^6Li as a specific example with a rather large mass ratio. If we take $\beta = (m_{\text{Li}} \omega_{\text{Li}}^2)/(m_{\text{Rb}} \omega_{\text{Rb}}^2) = 0.4$ (which means that $\omega_{\text{Li}} = 2.41 \times \omega_{\text{Rb}}$) we have $\Omega = 1.14 \times \omega_{\text{Rb}}$, $\omega = 2.34 \times \omega_{\text{Rb}}$, and $C = -0.877 \mu \omega^2$ from (7). Taking the harmonic oscillator length scale as an estimate of the magnitude of the dipole matrix elements, we can get the following order of magnitude estimate of the energy shift of the lowest energy states caused by the coupling:

$$\frac{|\Delta E|}{\hbar \omega} \sim \frac{|C|}{\hbar \omega} \sqrt{\frac{\hbar}{M \Omega}} \sqrt{\frac{\hbar}{\mu \omega}} = \frac{|C|}{\mu \omega^2 \sqrt{(M/\mu)(\Omega/\omega)}} = 0.3 \quad (8)$$

so the coupling is expected to be significant but the product basis is still a good starting point for our analysis.

We shall assume that the interaction potential is central, i.e., it is independent of the relative angular orientation of the atoms. This implies that the H_{cm} and H_{rel} commute with the angular momentum operators,

$$\mathbf{L} = \mathbf{R} \times \mathbf{P} \quad l = \mathbf{r} \times \mathbf{p} \quad (9)$$

where \mathbf{P} and \mathbf{p} are the conjugated momentum operators of \mathbf{R} and \mathbf{r} respectively and we can choose as basis for our description the product states

$$\psi_{NLMnlm}(\mathbf{R}, \mathbf{r}) = \Phi_{NLM}(\mathbf{R}) \varphi_{nlm}(\mathbf{r}) \quad (10)$$

where N and n are principal quantum numbers and L, M and l, m are the angular momentum quantum numbers of the CM and relative motion respectively. It is interesting to note that the total angular momentum of the particles $\mathbf{J} = \mathbf{l}_1 + \mathbf{l}_2$ can also be written as

$$\mathbf{J} = \mathbf{L} + l. \quad (11)$$

Since both H_{CM} , H_{rel} and $\mathbf{R} \cdot \mathbf{r}$ are rotationally invariant, the total angular momentum commutes with the full Hamiltonian, and our Hilbert space separates into independent subspaces belonging to different values of J and m_J which makes it natural to switch from the $|NLMnlm\rangle$ basis to the coupled $|Jm_J N L n l\rangle$ basis:

$$\psi_{N L n l}^{J m_J} = \sum_{M m} \langle L M l m | J m_J \rangle \Phi_{N L M}(\mathbf{R}) \varphi_{n l m}(\mathbf{r}) \quad (12)$$

where $\langle L M l m | J m_J \rangle$ denote the Clebsch Gordan coefficients.

To diagonalize the $\mathbf{R} \cdot \mathbf{r}$ coupling term in the basis (12) we need the matrix elements:

$$\begin{aligned} & \langle \psi_{N' L' n' l'}^{J m_J} | \mathbf{R} \cdot \mathbf{r} | \psi_{N L n l}^{J m_J} \rangle \\ &= \sum_{M' m' M m} \langle L' M' l' m' | J m_J \rangle \langle L M l m | J m_J \rangle \\ & \times \langle \Phi_{N' L' M'}(\mathbf{R}) \varphi_{n' l' m'}(\mathbf{r}) | \mathbf{R} \cdot \mathbf{r} | \Phi_{N L M}(\mathbf{R}) \varphi_{n l m}(\mathbf{r}) \rangle \end{aligned} \quad (13)$$

It should be emphasized that $\mathbf{R} \cdot \mathbf{r}$ does *not* commute with \mathbf{L}^2 and \mathbf{l}^2 so L and l are not good quantum numbers when the coupling term is included into the Hamiltonian. This is in contrast to, e.g., the $\mathbf{L} \cdot \mathbf{S}$ (spin-orbit) coupling in the hydrogen atom which commutes with L^2 and S^2 leaving L and S as good quantum numbers.

III. EIGENSTATES OF RELATIVE MOTION

A. Pseudopotential description

At sufficiently low temperatures atoms interact mainly through s-wave scattering since the centrifugal barrier for higher partial waves becomes much larger than the thermal energies. The interaction depends to a large extent

only on a single parameter, the s-wave scattering length a_{sc} , and the real physical interaction can be modelled by the following pseudopotential [19, 20]

$$V_{\text{int}}(r) = \frac{2\pi\hbar^2 a_{sc}}{\mu} \delta^{(3)}(\mathbf{r}) \frac{\partial}{\partial r} r \quad (14)$$

where the action of the operator $(\partial/\partial r)r$ on a wave function ψ is to be understood as $(\partial/\partial r)(r\psi)$. The pseudopotential reproduces the correct wave function in the entire range outside the range of the physical interaction.

Writing $u(r) = r\psi(r)$, the pseudopotential (14) implies the boundary condition [21],

$$\frac{u'(0)}{u(0)} = \frac{-1}{a_{sc}} \quad (15)$$

instead of the usual $u(0) = 0$ in a regular potential.

For interatomic potentials containing a long range van der Waals ($V(r) = -C_6/r^6$) attraction, the validity of the pseudopotential description for trapped atoms in a harmonic oscillator is determined by the ratio β_6/a_{ho} where $\beta_6 = (2\mu C_6/\hbar^2)^{1/4}$ is the characteristic potential length scale and $a_{ho} = \sqrt{\hbar/\mu\omega}$ is the length scale of the harmonic confining potential [22, 23]. Values of C_6 for both homonuclear and heteronuclear alkali metal atom pairs can be found in [24]. In the case of an optical lattice well with a trapping frequency of $\omega_{Rb} = 2\pi \times 200$ kHz we have $a_{ho} = 1.2 \times 10^3 a_0$ and since $\beta_6 = 85 a_0$ for $^{87}\text{Rb}-^6\text{Li}$ [24] we expect the pseudopotential approximation to be reasonably good even for a very tightly confining lattice.

The real interaction potential accommodates several bound states, but here we are only concerned with the very loosely bound state which can be accessed in Feshbach resonance experiments and this bound state is accounted for by the pseudopotential. The parameter which is used to tune the scattering length in experiments is the magnitude of the magnetic field B . Near a Feshbach resonance the scattering length is given by [25]

$$a_{sc} = a_{bg} \left(1 - \frac{\Delta}{B - B_0} \right) = a_{bg} \left(1 - \left(\frac{B - B_0}{\Delta} \right)^{-1} \right) \quad (16)$$

so if everything is expressed in terms of the dimensionless magnetic field $(B - B_0)/\Delta$ the only tunable parameters in the pseudopotential model are the harmonic oscillator frequency ω and the background scattering length a_{bg} (notice, however, that Δ might be negative).

Calculations of spectra in models with more accurate potentials can be found in [22, 26, 27], and pseudopotential models with an energy dependent scattering length have been used to improve the accuracy [22, 23]. While the exact spectra and matrix elements might be slightly different due to the limitations of our approximation, the pseudopotential captures the essential physics quite well and it gives good quantitative agreement in most cases.

B. Wave functions of relative motion

In this section we obtain solutions to the Schrödinger equation of the relative motion with the Hamiltonian (6) and the pseudopotential (14). These solutions, i.e., the energy spectrum and the wave functions have been provided previously [21, 28], but we give them here for completeness, as we shall use their precise form to subsequently evaluate the matrix elements of the coupling term $C\mathbf{R} \cdot \mathbf{r}$.

Let us first, for reference provide the spectrum

$$E = \hbar\omega \left(2n + l + \frac{3}{2} \right) \quad (17)$$

and the associated eigenfunctions

$$\begin{aligned} \psi_{nlm}(\mathbf{r}) & \\ &= \sqrt{\frac{2n!}{\Gamma(n+l+3/2)}} L_n^{l+1/2}(r^2) r^l e^{-r^2/2} Y_{lm}(\theta, \phi), \end{aligned} \quad (18)$$

for the three-dimensional isotropic harmonic oscillator. L_n^α are generalized Laguerre polynomials, r is given in units of the harmonic oscillator length $\sqrt{\hbar/(\mu\omega)}$, and Y_{lm} are the spherical harmonic wave functions.

The pseudopotential (14) only alters the solutions with $l = 0$ [28]. In the region $r > 0$ the radial Schrödinger equation, expressed in units of the harmonic oscillator length scale $a_{ho} = \sqrt{\hbar/\mu\omega}$ and energy scale $E = \hbar\omega\epsilon$, reads

$$-\frac{1}{2} \frac{\partial^2 u}{\partial r^2} + \frac{1}{2} r^2 u = \epsilon u \quad (20)$$

or

$$\frac{\partial^2 u}{\partial (\sqrt{2}r)^2} - \left(\frac{1}{4} (\sqrt{2}r)^2 - \epsilon \right) u = 0 \quad (21)$$

According to [29] 19.3.7 and 19.3.8, the solutions to this equation are the parabolic cylinder functions $D_{\epsilon-1/2}(\sqrt{2}r)$ and $V(-\epsilon, \sqrt{2}r)$ with the following asymptotic behaviour for large r ([29] 19.8.1 and 19.8.2):

$$D_{\epsilon-1/2}(\sqrt{2}r) \simeq e^{-r^2/2} (\sqrt{2}r)^{\epsilon-1/2} \quad (22)$$

$$V(-\epsilon, \sqrt{2}r) \simeq \sqrt{\frac{2}{\pi}} e^{r^2/2} (\sqrt{2}r)^{-\epsilon-1/2}. \quad (23)$$

The diverging V function must be discarded. The D function satisfies ([29] 19.3.5 and 19.3.7)

$$D_{\epsilon-1/2}(0) = \frac{\sqrt{\pi}}{2^{-\epsilon/2+1/4} \Gamma(-\epsilon/2+3/4)} \quad (24)$$

$$D'_{\epsilon-1/2}(0) = \frac{-\sqrt{\pi}}{2^{-\epsilon/2-1/4} \Gamma(-\epsilon/2+1/4)} \quad (25)$$

Normally we would only accept the regular solutions with $u(0) = 0$, which implies that the Γ function in (24) is

infinite, and hence that its argument is a non-positive integer. Thus, $\epsilon = 2n + 3/2$ where $n = 0, 1, 2, \dots$ in agreement with (17). The pseudopotential (14), however, imposes the boundary condition (15), and the discrete energy spectrum ϵ_ν is given by the solutions to the following transcendental equation:

$$\frac{\sqrt{2}D'_{\epsilon-1/2}(0)}{D_{\epsilon-1/2}(0)} = \frac{-2\Gamma(-\epsilon/2 + 3/4)}{\Gamma(-\epsilon/2 + 1/4)} = \frac{-a_{\text{ho}}}{a_{\text{sc}}}$$

It is convenient to associate to each eigenenergy an effective harmonic oscillator quantum number ν defined by

$$\epsilon = 2\nu + \frac{3}{2} \quad (26)$$

such that $u(r) \propto D_{2\nu+1}(\sqrt{2}r)$ and

$$\psi_\nu(\mathbf{r}) = \frac{u_\nu(r)}{r} Y_{00} = \frac{N_\nu}{r} 2^{-\nu-1/2} D_{2\nu+1}(\sqrt{2}r) Y_{00} \quad (27)$$

where

$$N_\nu = \sqrt{\frac{2\Gamma(-\nu - 1/2)\Gamma(-\nu)}{\pi[\psi(-\nu) - \psi(-\nu - 1/2)]}} \quad (28)$$

is a normalization constant and ψ is the digamma function (see Appendix). The wave function generally diverges as $1/r$ for small r since $u(0)$ is generally finite according to (24). The expression (27) can also be rewritten in terms of the confluent hypergeometric U function (see [29] 13.6.36 and 13.1.29) to obtain the forms cast in [21, 28].

C. Dipole matrix elements and non-separable eigenstates

In a given Jm_J subspace the matrix representation of the Hamiltonian (4) in the $|N L \nu l\rangle$ basis, abbreviated by state indices p, q , is the sum of diagonal contributions from H_{CM} and H_{rel} and an off-diagonal contribution from the coupling term $C\mathbf{R} \cdot \mathbf{r}$ (see Eq. 13):

$$\begin{aligned} H_{pq} &= \hbar\Omega(2N_p + L_p + 3/2)\delta_{pq} + \hbar\omega(2\nu_p + l_p + 3/2)\delta_{pq} \\ &+ C \sum_{M_p m_p M_q m_q} \langle L_p M_p l_p m_p | J m_J \rangle \langle L_q M_q l_q m_q | J m_J \rangle \\ &\times \langle \Phi_{N_p L_p M_p}(\mathbf{R}) | \mathbf{R} | \Phi_{N_q L_q M_q}(\mathbf{R}) \rangle_{\mathbf{R}} \\ &\cdot \langle \varphi_{\nu_p l_p m_p}(\mathbf{r}) | \mathbf{r} | \varphi_{\nu_q l_q m_q}(\mathbf{r}) \rangle_{\mathbf{r}} \end{aligned} \quad (29)$$

where $\langle \rangle_{\mathbf{R}}$ and $\langle \rangle_{\mathbf{r}}$ denote integration with respect to \mathbf{R} , respectively \mathbf{r} and δ_{pq} is the Kronecker delta.

The dipole integrals separate into radial and angular components. The radial dipole integral for harmonic oscillator wave functions is given by the following simple formula, see Appendix:

$$\begin{aligned} \int_0^\infty R_{N'(L+1)}(r) r R_{NL}(r) r^2 dr \\ = \sqrt{N+L+3/2} \delta_{N',N} - \sqrt{N} \delta_{N',N-1} \end{aligned} \quad (30)$$

The parabolic cylinder wave functions have $l = 0$ so they couple only to the $l = 1$ harmonic oscillator states. In the Appendix we denote the radial parts of the wave functions by R_ν and R_{n1} , and we derive

$$\begin{aligned} \int_0^\infty R_\nu(r) r R_{n1}(r) r^2 dr \\ = N_\nu \sqrt{\frac{2n!}{\Gamma(n+5/2)}} \frac{\sqrt{\pi}}{16} \\ \times \sum_{k=0}^n 2^{-2k} (-1)^k \binom{n+\alpha}{n-k} \frac{1}{k!} \frac{\Gamma(2k+4)}{\Gamma(k+2-\nu)}. \end{aligned} \quad (31)$$

We now have analytical expressions for the full Hamiltonian matrix. Consider the case where the system is prepared, and therefore remains, in the block of $J = 0, m_J = 0$ states. Such states involve CM and relative states with $L = l$ and $M = -m$ and using the Clebsch-Gordan coefficient $\langle LMlm | J = 0, m_J = 0 \rangle = \delta_{M(-m)} (-1)^{L-M} / \sqrt{2L+1}$ we have

$$\begin{aligned} \psi_{N L n L}^{00}(\mathbf{R}, \mathbf{r}) \\ = \frac{1}{\sqrt{2L+1}} \sum_{M=-L}^L (-1)^{L-M} \Phi_{N L M}(\mathbf{R}) \varphi_{n L (-M)}(\mathbf{r}). \end{aligned} \quad (32)$$

When we diagonalize the Hamiltonian in the basis (32) we get the $J = 0$ spectrum shown in Fig. 1. Note that we plot the energies as functions of scattering length, which in turn must be described as a function of the magnetic field in an experiment.

As the eigenfunctions Ψ of the complete Hamiltonian are expanded on the basis (32) of angular momentum eigenstates

$$\Psi = \sum_{N L n} c_{N L n} \psi_{N L n}^{00} \quad (33)$$

the expansion coefficients provide, through $|c_{N L n}|^2$, the CM and relative angular momentum content of the eigenstates. We observe that with a central interaction potential and spherically symmetric single-particle confining potentials, it is possible to generate states with non-vanishing relative, and center-of-mass, angular momenta. In Tab. I and in Tab. II the population of different angular momentum components are given for the lowest eigenstates of the system for $a_{\text{sc}} = 0$ and for $a_{\text{sc}}/a_{\text{ho}} = 0.36$. For instance the state with an energy of $3.64 \hbar\omega$ at $a_{\text{sc}} = 0$ contains 63.2 % of $|010\rangle$ with $L = l = 1$, 13.6 % of $|100\rangle$ with $L = l = 0$, and 23.1 % of other product states.

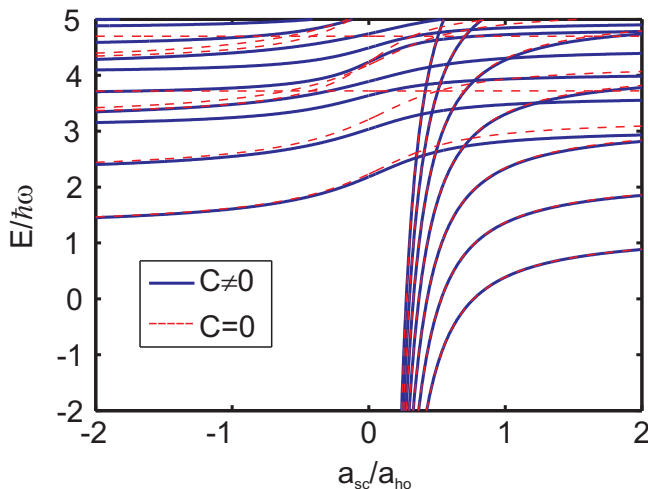


Figure 1: (Color online) $J = 0$ spectrum of a Rb and a Li atom in a harmonic well in the pseudopotential approximation. The energy scale $\hbar\omega$ of the relative motion harmonic oscillator is chosen as the unit of energy. $\beta = (m_{\text{Li}}\omega_{\text{Li}}^2)/(m_{\text{Rb}}\omega_{\text{Rb}}^2) = 0.4$. The spectrum of the full Hamiltonian including the coupling between CM and relative dynamics is shown as the connected, blue lines. The spectrum we get before including the coupling term is shown as red, dashed lines. We have included states up to $N = 6$, $n = 6$ and $L = l = 12$ which gives a total of 637 product basis states. Note the equidistant CM vibrational states of molecular nature when $a_{\text{sc}} > 0$.

Energy	Largest content		Second largest content	
	$ N Ln\rangle$	$ c_{N Ln} ^2$ (%)	$ N Ln\rangle$	$ c_{N Ln} ^2$ (%)
2.18	$ 000\rangle$	96.2	$ 010\rangle$	3.5
3.04	$ 100\rangle$	79.1	$ 010\rangle$	11.2
3.64	$ 010\rangle$	63.2	$ 100\rangle$	13.6
3.89	$ 200\rangle$	64.0	$ 110\rangle$	16.7
4.24	$ 001\rangle$	80.8	$ 010\rangle$	12.6
4.49	$ 110\rangle$	33.5	$ 200\rangle$	22.8
4.74	$ 300\rangle$	51.1	$ 210\rangle$	18.3

Table I: Angular momentum basis content at $a_{\text{sc}} = 0$ of the eigenstates of the full Hamiltonian for ^{87}Rb and ^6Li in a harmonic potential with $\beta = (m_{\text{Li}}\omega_{\text{Li}}^2)/(m_{\text{Rb}}\omega_{\text{Rb}}^2) = 0.4$.

IV. RESONANT DYNAMICS NEAR A FESHBACH RESONANCE

A recent experiment [8] has demonstrated the formation of heteronuclear molecules by RF association from another hyperfine state near a Feshbach resonance in the ^{87}Rb - ^{40}K system.

Extending our previous work [18] for identical systems we will now address the dynamics beyond the adiabatic approximation, where a modulation of the field causes transitions *between* the adiabatic eigenstates. As a specific application we will discuss resonant transitions driven by an oscillating magnetic field. The idea, proposed and used by Thompson et al. [30] and Greiner et al. [31] and theoretically analyzed in [18, 32], is to apply

Energy	Largest content		Second largest content	
	$ N Ln\rangle$	$ c_{N Ln} ^2$ (%)	$ N Ln\rangle$	$ c_{N Ln} ^2$ (%)
-3.09	$ 000\rangle$	99.997	$ 010\rangle$	0.0013
-2.12	$ 100\rangle$	99.994	$ 110\rangle$	0.002
-1.14	$ 200\rangle$	99.990	$ 210\rangle$	0.003
-0.16	$ 300\rangle$	99.985	$ 310\rangle$	0.004
0.81	$ 400\rangle$	99.981	$ 410\rangle$	0.005
1.79	$ 500\rangle$	99.977	$ 410\rangle$	0.006
2.53	$ 001\rangle$	91.0	$ 010\rangle$	8.0
2.76	$ 600\rangle$	99.973	$ 510\rangle$	0.008
3.29	$ 101\rangle$	58.7	$ 010\rangle$	22.0
3.81	$ 010\rangle$	58.9	$ 101\rangle$	21.7
4.11	$ 201\rangle$	43.8	$ 110\rangle$	18.8
4.57	$ 002\rangle$	64.0	$ 011\rangle$	17.1
4.71	$ 110\rangle$	26.4	$ 201\rangle$	16.9
4.93	$ 301\rangle$	30.6	$ 201\rangle$	17.2

Table II: Angular momentum basis content at $a_{\text{sc}} = 0.36\sqrt{\hbar/\mu\omega}$ of the eigenstates of the full Hamiltonian for ^{87}Rb and ^6Li in a harmonic potential with $\beta = (m_{\text{Li}}\omega_{\text{Li}}^2)/(m_{\text{Rb}}\omega_{\text{Rb}}^2) = 0.4$. The molecular states are almost pure product states with $n = 0$, $L = 0$ and a well defined CM excitation N whereas for all other states the CM dynamics and the relative dynamics are entangled.

small sinusoidal oscillations of the magnetic field around a fixed value B' close to a Feshbach resonance:

$$B(t) = B' + b \sin(\omega_B t). \quad (34)$$

If $\hbar\omega_B$ matches the energy difference between two stationary states, it is possible to transfer population from one state to another (for instance to the molecular state) or to create well controlled quantum mechanical superposition states.

The modulation technique has also been used to produce and make spectroscopy on ultracold heteronuclear ^{87}Rb - ^{85}Rb molecules [33], to probe the excitation spectrum of a Fermi gas in the BEC-BCS crossover regime [31], and to infer the lifetime of short-lived Feshbach molecules by looking at the width of the resonance [34]. It differs in principle from the traditional RF spectroscopy used in e.g. [7, 35, 36] in that the atoms are not transferred to other hyperfine levels and in that it is the tunable interatomic interaction that drives the transition.

When the magnetic field is varied in time, the interaction Hamiltonian is explicitly time dependent, and we have different options to determine the evolution of the system.

A. Weak amplitude modulations of B-field

If the B-field modulation is weak, it constitutes only a small time-dependent perturbation on the system, and a calculation naturally departs from an expansion in the adiabatic eigenstate basis. We label the complete set of eigenstates of the Hamiltonian at a given field strength by $|\Psi_q(B)\rangle$ and their energies E_q , and we expand the

wave function $|\Psi(t)\rangle$

$$|\Psi(t)\rangle = \sum_q c_q(t) |\Psi_q(B(t))\rangle \quad (35)$$

Inserting into the time-dependent Schrödinger equation, and projecting onto the orthogonal states $\langle\Psi_p(B(t))|$ we get the coupled amplitude equations

$$\begin{aligned} i\hbar \frac{dc_p(t)}{dt} &= E_p(t)c_p(t) \\ &- i\hbar \sum_q \frac{\partial}{\partial t'} \langle\Psi_p(B(t))|\Psi_q(B(t'))\rangle \Big|_{t'=t} c_q(t). \end{aligned} \quad (36)$$

If we take the sinusoidal magnetic field dependence (34) in (36) we get the following equation for the coefficients

$$i\hbar \frac{dc_p(t)}{dt} = E_p(t)c_p(t) - i\hbar \cos(\omega_B t) \sum_q \Omega_{pq}(B(t)) c_q(t). \quad (37)$$

where the Rabi frequencies Ω_{pq} are given by

$$\Omega_{pq}(B) = b\omega_B \frac{\partial}{\partial B'} \langle\Psi_p(B)|\Psi_q(B')\rangle \Big|_{B'=B}. \quad (38)$$

For a weakly modulated field, $b \ll \Delta$, the time dependence of E_p and Ω_{pq} can be neglected and the modulation is equivalent to, e.g., the radiative coupling of atomic energy levels. If $\hbar\omega_B$ is close to the energy difference between two eigenstates p and q , and we have all the population in the states p initially, we therefore expect to see Rabi oscillations between the two states

$$|c_q(t)|^2 = 1 - |c_p(t)|^2 = \left(\frac{\Omega_{pq}}{\Omega'_{pq}}\right)^2 \sin^2\left(\frac{\Omega'_{pq}}{2} t\right) \quad (39)$$

where

$$\Omega'_{pq} = \sqrt{\Omega_{pq}^2 + (\omega_B - (E_p - E_q)/\hbar)^2}. \quad (40)$$

B. General dynamical equations in modulated B-field

The expansion (35) is general and may be applied for any modulation of the magnetic field, but since the eigenstates in that expansion have to be found first by numerical diagonalization of the coupling Hamiltonian, we find it more convenient to use instead the basis (12), where only the relative coordinate part of the wave function depends explicitly on time through the scattering length. We then get

$$i\hbar \frac{dc_p(t)}{dt} \quad (41)$$

$$= \sum_q H_{pq}(t)c_q(t) - i\hbar \sum_q \frac{\partial}{\partial t'} \langle\psi_p(t)|\psi_q(t')\rangle \Big|_{t'=t} c_q(t) \quad (42)$$

where H_{pq} is given in (29).

The explicit expression for the time derivative of $\langle\psi_p(t)|\psi_q(t')\rangle$ in the basis (12) is

$$\begin{aligned} &\frac{\partial}{\partial t'} \langle\psi_p(t)|\psi_q(t')\rangle \Big|_{t'=t} \\ &= \sum_{M_p m_p M_q m_q} \langle L_p M_p l_p m_p | J m_J \rangle \langle L_q M_q l_q m_q | J m_J \rangle \\ &\quad \times \langle \Phi_{N_p L_p M_p} | \Phi_{N_q L_q M_q} \rangle_{\mathbf{R}} \\ &\quad \times \frac{\partial}{\partial t'} \langle \varphi_{n_p l_p m_p}(t) | \varphi_{n_q l_q m_q}(t') \rangle_{\mathbf{r}} \Big|_{t'=t} \end{aligned} \quad (43)$$

where we have exploited the fact that only the relative coordinate wave function φ is time dependent. We note that our use of the adiabatic eigenfunctions of H_{rel} removes the need to numerically compute any matrix elements of the singular interaction potential, and thus we make optimum use of our knowledge of the analytical, irregular solutions to the pseudopotential equation.

It is a great advantage of the pseudopotential model that the matrix element $\langle\varphi_{\nu 00}|\varphi_{\nu' 00}\rangle$ can be calculated analytically, and we can hence express the time derivative using the chain rule:

$$\begin{aligned} &\frac{\partial}{\partial t'} \langle\varphi_{n_p 00}(t) | \varphi_{n_q 00}(t')\rangle_{\mathbf{r}} \Big|_{t'=t} \\ &= \frac{dB}{dt} \frac{da_{\text{sc}}}{dB} \left(\frac{da_{\text{sc}}}{d\nu'}\right)^{-1} \frac{\partial}{\partial \nu'} \langle\varphi_{\nu_p 00} | \varphi_{\nu' 00}\rangle_{\mathbf{r}} \Big|_{\nu'=\nu_q} \end{aligned} \quad (44)$$

where da_{sc}/dB is given by

$$\frac{da_{\text{sc}}}{dB} = \frac{-\Delta}{(B - B_0)^2} a_{\text{bg}}, \quad (45)$$

and $da_{\text{sc}}/d\nu$ is given by

$$\frac{da_{\text{sc}}}{d\nu} = \frac{a_{\text{sc}}}{[f(\nu)]^2} = \frac{a_{\text{bg}}}{[f(\nu)]^2} \frac{B - B_0 - \Delta}{B - B_0} \quad (46)$$

with

$$f(\nu) = \frac{1}{\sqrt{\psi(-\nu) - \psi(-\nu - \frac{1}{2})}}. \quad (47)$$

The overlap $\langle\varphi_{\nu 00}|\varphi_{\nu' 00}\rangle$ is provided in the Appendix and all coefficients in our coupled set of equations are thus given by analytical expressions.

C. Results

According to the discussion in Sec. IV A a small amplitude harmonic oscillation of the magnetic field at a frequency such that $\hbar\omega$ is resonant with the energy difference between two eigenstates will inevitably lead to

full contrast Rabi oscillations as long as there is a finite coupling between the two states. For $\mathbf{J} = 0$ such a finite coupling arises whenever the basis expansion (33) of the two eigenstates at the given magnetic field B' contains basis functions of the form $\Phi_{N00}(\mathbf{R})\varphi_{\nu'00}(\mathbf{r})$ respectively $\Phi_{N00}(\mathbf{R})\varphi_{\nu'00}(\mathbf{r})$, see Eq. 43.

This means e.g. that efficient association of heteronuclear molecules should be possible. We can illustrate it in principle using the ^{87}Rb - ^6Li system treated above. The scattering length at zero magnetic field was measured by C. Silber et al. [37] to be $20(+9/-6) a_0$. A Feshbach resonance with this background scattering length gives rise to the energy spectrum shown in Fig. 2. If we oscillate the magnetic field resonantly around $B = B_0 - 0.05\Delta$ (corresponding to $a_{sc}/a_{ho} = 0.36$) we can produce full contrast Rabi oscillations between the lowest non-molecular state and the molecular ground state (illustrated with the lowermost arrow in the spectrum). The dynamics is shown in Fig. 3. In practise one might want to use an adiabatic passage to make a robust full transfer as demonstrated in [18].

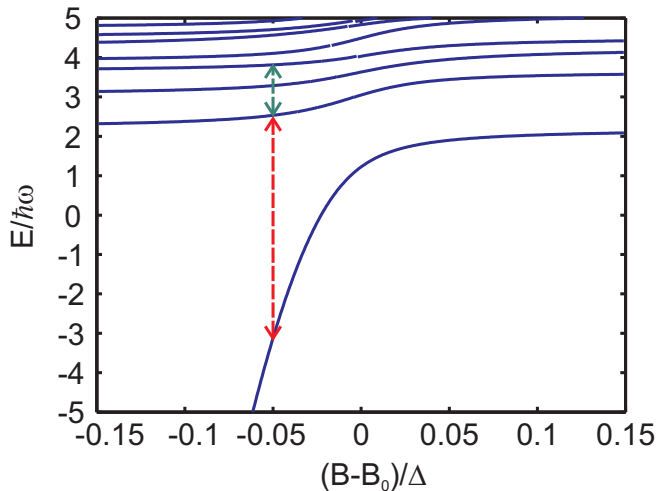


Figure 2: (Color online) Spectrum for ^{87}Rb - ^6Li in an optical lattice well with $\omega_{\text{Rb}} = 2\pi \times 200$ kHz and $\beta = m_{\text{Li}}\omega_{\text{Li}}^2/(m_{\text{Rb}}\omega_{\text{Rb}}^2) = 0.4$ in the vicinity of a Feshbach resonance with $a_{\text{bg}} = 20 a_0$. Molecular states that have a CM excitation ($N > 0$) are not shown. Association of a heteronuclear molecule is indicated with the lower, red arrow while transfer to a state with angular momentum excitation is illustrated with the upper, green arrow.

Another interesting fact is that the coupling of the CM and relative motion makes it possible to populate states with nonzero CM and relative angular momentum by oscillating the magnetic field close to a Feshbach resonance. It is intriguing that in this way a purely central interatomic interaction can be used to put angular momentum into the relative motion at the cost of exciting the CM motion as well.

For example the uppermost arrow in Fig. 2 illustrates a transfer from the non-molecular atomic ground state to a

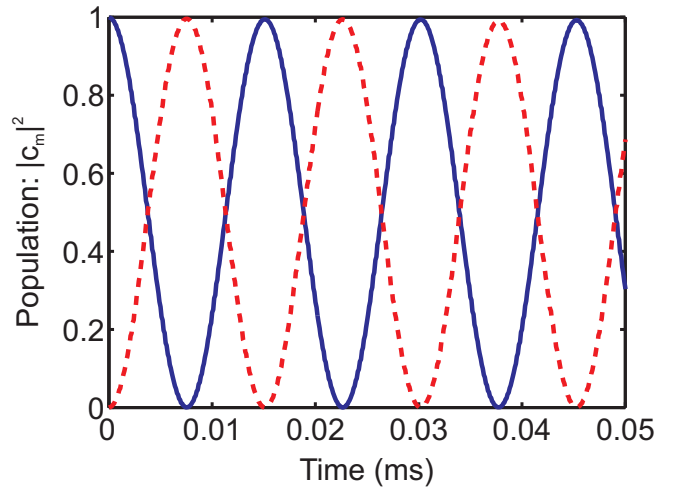


Figure 3: (Color online) Resonant association of heteronuclear molecules by an oscillating magnetic field. The time dependent magnetic field is $B(t) = B_0 - 0.05\Delta + 0.005\Delta \sin(\omega_B t)$ where $\omega_B = 2\pi \times 2660$ kHz. The blue line shows the population of the atomic ground state whereas the population of the molecular ground state is shown with the red, dashed line. $\omega_{\text{Rb}} = 2\pi \times 200$ kHz, $\beta = m_{\text{Li}}\omega_{\text{Li}}^2/(m_{\text{Rb}}\omega_{\text{Rb}}^2) = 0.4$. We have included states up to $N = 3$, $n = 3$ and $L = l = 6$.

state with 59 % content of $L = l = 1$ (see Tab. II). If the magnetic field is oscillated resonantly, Rabi oscillations between these two states can be produced (Fig. 4) and again a π -pulse or an adiabatic passage could in principle be used to make a full transfer.

V. DISCUSSION

In summary, we have found the eigenstates of motion of a pair of harmonically trapped, different atoms interacting via a short range central potential. We have investigated the dynamics of the system when the interaction strength is modulated, by changing the strength of an applied magnetic field, and in particular we have found that resonant transitions between the molecular and atomic states can be coherently driven in this system. Interestingly we find that even though the interaction is central, states with non-vanishing CM and relative angular momentum of the atoms can be produced. Although our calculations were done explicitly for the pseudo-potential (14), this is not a formal restriction on the separation of the problem and the methods applied, and other central interaction potentials are readily treated by a similar analysis.

We believe that the transition dynamics analyzed in the present paper may be studied with current experimental techniques. Our work identifies a way to produce molecules without crossing the Feshbach resonance, and we imagine that the states with nonvanishing relative angular momentum may lead to interesting momentum

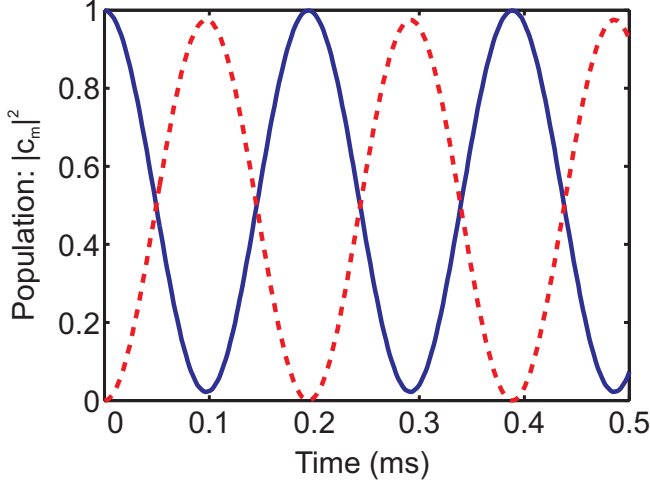


Figure 4: (Color online) Rabi oscillations between the atomic ground state and a state with 59 % content of $L = l = 1$. The time dependent magnetic field is $B(t) = B_0 - 0.05\Delta + 0.005\Delta \sin(\omega_B t)$ where $\omega_B = 2\pi \times 601$ kHz. The blue line shows the population of the atomic ground state whereas the population of the excited angular momentum state is shown with the red, dashed line. The other parameters are as in Fig. 3.

distributions [38, 39, 40] of the individual species when the atoms are released from the lattice.

Acknowledgments

We gratefully acknowledge discussions with Michael Budde, Nicolai Nygaard and Ejvind Bonderup.

VI. APPENDIX: CALCULATION OF MATRIX ELEMENTS

This appendix derives the matrix elements used in the Feshbach molecule problem. We consider the radial wave functions for an isotropic 3-dimensional harmonic oscillator (18)

$$R_{nl}(r) = N_{nl} L_n^{l+1/2}(r^2) r^l e^{-r^2/2} \quad (48)$$

where L is a generalized Laguerre polynomial, and the s-wave solutions to the problem of a particle in a harmonic oscillator modified by a regularized s-wave δ -function potential at the origin (27)

$$R_\nu(r) = \frac{N_\nu}{r} 2^{-\nu-1/2} D_{2\nu+1}(z), \quad z = \sqrt{2}r \quad (49)$$

where D is the parabolic cylinder function. N_{nl} and N_ν are normalization constants.

A. Radial integral for harmonic oscillator wave functions

The normalization constant of the harmonic oscillator wave functions is given by

$$\begin{aligned} \frac{1}{N_{nl}^2} &= \int_0^\infty \left[L_n^{l+1/2}(r^2) \right]^2 r^{2l+2} e^{-r^2} dr \\ &= \frac{1}{2} \int_0^\infty \left[L_n^{l+1/2}(u) \right]^2 u^{l+1/2} e^{-u} du \\ &= \frac{\Gamma(n+l+3/2)}{2n!} \end{aligned} \quad (50)$$

where we have used ([29] 22.2.12, [41] 7.414.3):

$$\begin{aligned} \int_0^\infty e^{-x} x^\alpha L_n^\alpha(x) L_m^\alpha(x) dx \\ = \begin{cases} \frac{\Gamma(\alpha+n+1)}{n!}, & m = n, \text{Re } \alpha > 0 \\ 0, & m \neq n, \text{Re } \alpha > -1 \end{cases} \end{aligned} \quad (51)$$

The radial part of the dipole matrix element between oscillator states involves the integral

$$\begin{aligned} \int_0^\infty L_{n'}^{l'+1/2}(r^2) L_n^{l+1/2}(r^2) r^{l'+l+3} e^{-r^2} dr \\ = \frac{1}{2} \int_0^\infty L_{n'}^{l'+1/2}(u) L_n^{l+1/2}(u) u^{(l'+l+2)/2} e^{-u} du \end{aligned} \quad (52)$$

Since the angular integral has the selection rule $|\Delta l| = 1$ we can, without loss of generality, assume that $l' = l + 1$ and employ the recursion relation

$$L_n^{\alpha-1}(u) = L_n^\alpha(u) - L_{n-1}^\alpha(u) \quad (53)$$

for the generalized Laguerre polynomials ([29] 22.7.30) to obtain

$$\begin{aligned} \frac{1}{2} \int_0^\infty L_{n'}^{l'+1/2}(u) L_n^{l+1/2}(u) u^{(l'+l+2)/2} e^{-u} du \\ = \frac{1}{2} \int_0^\infty L_{n'}^{l+3/2}(u) \left(L_n^{l+3/2}(u) - L_{n-1}^{l+3/2}(u) \right) \\ \times u^{(2l+3)/2} e^{-u} du \\ = \frac{1}{2} \frac{\Gamma(n'+l+5/2)}{(n')!} (\delta_{n',n} - \delta_{n',n-1}) \end{aligned} \quad (54)$$

where (51) was used in the last step. Including the nor-

malization (50) we obtain

$$\begin{aligned}
& \int_0^\infty R_{n',l+1}(r)rR_{nl}(r)r^2dr \\
&= \sqrt{\frac{\Gamma(n'+l+5/2)}{\Gamma(n+l+3/2)} \frac{n!}{(n')!}} (\delta_{n',n} - \delta_{n',n-1}) \\
&= \sqrt{n+l+3/2} \delta_{n',n} - \sqrt{n} \delta_{n',n-1} \quad (55)
\end{aligned}$$

where the identity $\Gamma(x+1) = x \Gamma(x)$ has been used.

B. Radial overlap of parabolic cylinder functions

The normalization constant of the parabolic cylinder wave functions (49) is given by

$$\begin{aligned}
\frac{1}{N_\nu^2} &= \int_0^\infty R_\nu(r)^2 r^2 dr = 2^{-2\nu-1} \int_0^\infty [D_{2\nu+1}(z)]^2 \frac{dz}{\sqrt{2}} \\
&= 2^{-2\nu-3} \sqrt{\pi} \frac{\psi(-\nu) - \psi(-\nu - 1/2)}{\Gamma(-2\nu - 1)} \\
&= \frac{\pi}{2} \frac{\psi(-\nu) - \psi(-\nu - 1/2)}{\Gamma(-\nu - 1/2)\Gamma(-\nu)} \quad (56)
\end{aligned}$$

where [41] 7.711 has been used to solve the integral and the duplication formula for gamma functions [29] 6.1.18 has been used in the last equality. ψ is the digamma function:

$$\psi(x) = \frac{d}{dx} \ln \Gamma(x) = \frac{\Gamma'(x)}{\Gamma(x)}. \quad (57)$$

In the case $\nu' \neq \nu$ we apply [41] 7.711 to determine the overlap integral

$$\begin{aligned}
\langle \varphi_{\nu'} | \varphi_\nu \rangle &= N_{\nu'} N_\nu 2^{-\nu' - \nu - 1} \int_0^\infty D_{2\nu'+1}(z) D_{2\nu+1}(z) \frac{dz}{\sqrt{2}} \\
&= N_{\nu'} N_\nu \frac{\pi}{2(\nu' - \nu)} \left[\frac{1}{\Gamma(-\nu')\Gamma(-\nu - 1/2)} - \frac{1}{\Gamma(-\nu)\Gamma(-\nu' - 1/2)} \right] \\
&= \frac{f(\nu')f(\nu)}{\nu - \nu'} \times \frac{\Gamma(-\nu')\Gamma(-\nu - \frac{1}{2}) - \Gamma(-\nu)\Gamma(-\nu' - \frac{1}{2})}{\sqrt{\Gamma(-\nu' - \frac{1}{2})\Gamma(-\nu')} \sqrt{\Gamma(-\nu - \frac{1}{2})\Gamma(-\nu)}} \quad (58)
\end{aligned}$$

where

$$f(\nu) = \frac{1}{\sqrt{\psi(-\nu) - \psi(-\nu - \frac{1}{2})}} \quad (59)$$

C. Dipole matrix element between parabolic cylinder and harmonic oscillator p-wave functions

We evaluate

$$\begin{aligned}
& \int_0^\infty R_\nu(r) R_{n1}(r) r^3 dr \\
&= \int_0^\infty \left[\frac{N_\nu}{r} 2^{-\nu-1/2} D_{2\nu+1}(z) \right] \left[N_{n1} L_n^{3/2}(r^2) r e^{-r^2/2} \right] r^3 dr, \quad z^2 = 2r^2 \\
&= N_\nu N_{n1} 2^{-\nu-1/2} \int_0^\infty D_{2\nu+1}(z) L_n^{3/2}(z^2/2) \frac{z^3}{2^{3/2}} e^{-z^2/4} \frac{dz}{\sqrt{2}} \quad (60)
\end{aligned}$$

The generalized Laguerre polynomials are given by ([29] 22.3.9)

$$L_n^\alpha(u) = \sum_{k=0}^n a_k u^k, \quad a_k = (-1)^k \binom{n+\alpha}{n-k} \frac{1}{k!} \quad (61)$$

and we integrate term by term using ([41] 7.722 for $\mu > 0$):

$$\int_0^\infty e^{-x^2/4} x^{\mu-1} D_{-\tilde{\nu}}(x) dx = \frac{\sqrt{\pi} 2^{-\mu/2-\tilde{\nu}/2} \Gamma(\mu)}{\Gamma(\mu/2 + \tilde{\nu}/2 + 1/2)} \quad (62)$$

with $\tilde{\nu} = -(2\nu + 1)$ to get

$$\begin{aligned} & \int_0^\infty R_\nu(r) R_{n1}(r) r^3 dr \\ &= N_\nu N_{n1} \frac{\sqrt{\pi}}{16} \sum_{k=0}^n 2^{-2k} (-1)^k \binom{n+\alpha}{n-k} \frac{1}{k!} \frac{\Gamma(2k+4)}{\Gamma(k+2-\nu)}. \end{aligned} \quad (63)$$

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